Effects of plastic deformation on the optical properties of alkali halide and thallium halide single crystals

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EFFECTS OF PLASTIC DEFORMATION ON THE OPTICAL PROPERTIES OF ALKALI HALIDE AND THALLIUM HALIDE SINGLE CRYSTALS

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The effects of plastic deformation on the transmission of TlCl in the visible range, the static dielectric constant of TlCl, and the reflection spectra of NaF and TlCl corresponding to the restrahlen or residual ray were measured. The transmission and the static dielectric constant are decreased with the increasing deformation ratio. The effect of plastic deformation can not be found in the reflection spectrum of TlCl, but the decrease of reflectance of the side band and the splitting of the main band with the deformation are found in that of NaF.

Introduction

In the infrared reflection spectra of ionic crystals, there is a marked peak, corresponding to the restrahlen or residual rays. The frequency at this peak corresponds approximately to the fundamental optical mode of vibration. In the harmonic approximation when cyclic boundary conditions are employed, it can be shown that a very simple spectrum consisting of several bands of finite width indicates the inadequacy of this simple theory. The suggestions which have been proposed to explain this are the following: (1) use of free boundary conditions instead of cyclic boundary conditions[1]; (2) mechanical anharmonicity; (3) electrical anharmonicity[2~4]. From the temperature dependence of the lattice absorption of ionic crystals, the most probable model is supposed to be consistent with that assuming anharmonic forces[5]. For the analysis of these models, it is necessary to measure the other effects on the lattice absorption.

Mayburg[6] has measured the pressure dependence on the static dielectric constant of alkali halide, and found the reduction of the constant with increasing pressure.

In the present study, the effects and the contribution of the lattice imperfection produced by the plastic deformation of NaF and TlCl single crystals on the reflection spectrum corresponding restrahlen, the static dielectric constant and the optical absorption in the visible region are studied.

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Experimentals

The furnace used to produced the single crystals and the apparatus used to deform the crystals have been described in the previous papers[7,8]. The reflection spectra, the static dielectric constant and the optical absorption of the NaF and TlCl single crystals before deformation were measured by using the following apparatus. The reflection spectra corresponding restrahlen were measured by the vacuum grating spectrometer of much higher resolving power at Yoshinaga Laboratory, Faculty of Technology, Osaka University. The dielectric constants at the frequency of 1 Mc were measured by Q-meter, the Model Yokogawa QM-102. The absorption spectra were measured with the spectrometer, the Model Hitachi EPU-2A.

Results

As shown in Fig. 1, the absorptions of TlCl are increased with increasing deformation ratio, and the increases of absorption in the direction normal to the compression are larger than that

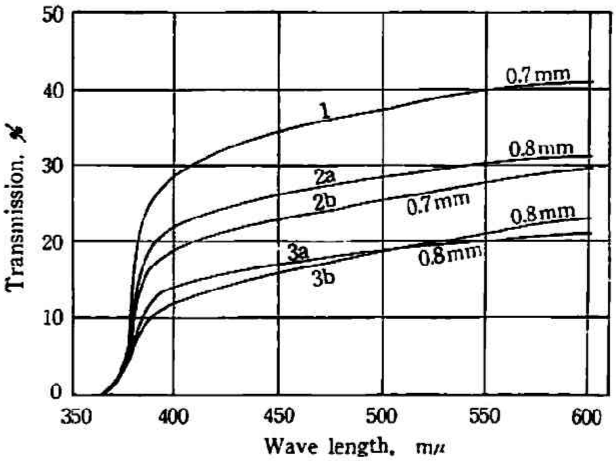

Fig. 1 Change of absorption spectra of TlCl crystal after plastic deformation
1: Absorption spectrum of the crystal measured before plastic deformation
2a and 2b: after 25% deformation
3a and 3b: after 50% deformation
a and b indicate the measurements in the directions parallel and normal to compression respectively.

Table The effect of plastic deformation on the static dielectric constant of thallium chloride

Deformation ratio, %	Direction of measurement	Dielectric constant (at 1 Mc)
0	press	31.47 (31.9)
	deform	〃
25	press	30.9
	deform	29.1
50	press	28.4
	deform	28.5

7) M. Ôura, *This Journal*, 30, 25 (1960)
8) M. Ôura, *ibid.*, 30, 92 (1960)

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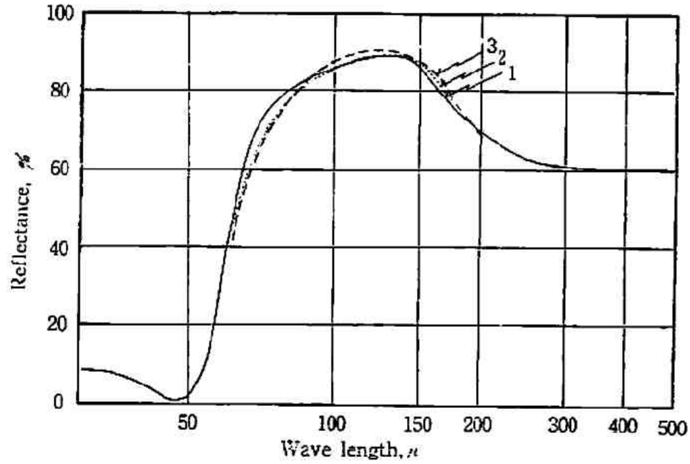

Fig. 2 Reflection spectra of TlCl crystal before and after deformation with a ratio 50%
1: before deformation
2, 3: after deformation measured in the direction normal and parallel to the compression respectively

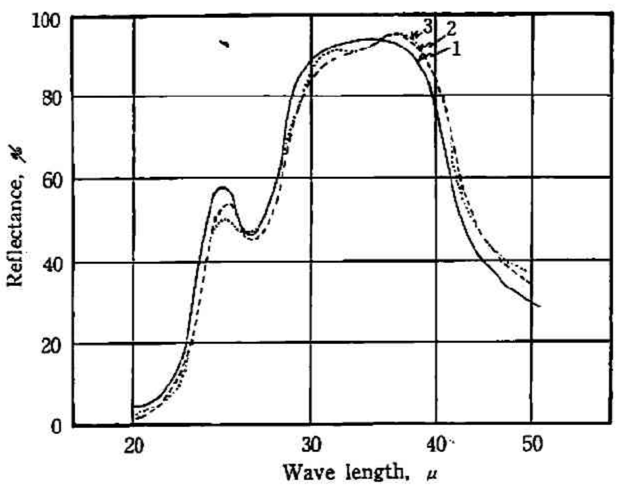

Fig. 3 Reflection spectra of NaF crystal before and after deformation with a ratio 25%
1: before deformation
2, 3: after deformation measured in the direction respectively

in the direction parallel. On the other hand, the static dielectric constants before and after deformation at 1 Mc are shown in Table. The static dielectric constants are decreased with increasing deformation ratio. But, as shown in Fig. 2, the effect of the deformation can not be found in the reflection spectra corresponding to the restrahlen of deformed TlCl crystal. On the other hand, the decrease of the reflectance of the side band is found in the 25% deformed NaF. The decrease of the side band is more remarkable in the spectrum measuren in the direction parallel to the compression than that in the direction normal.

Discussions

The increasing of the optical absorption in the visible region shown in Fig. 1 is supposed to be the result of the scattering of the incident rays by the lattice imperfection produced with the plastic deformation of the crystal.

The polarization in the ionic crystal which contributes to the static dielectric constant is separated into two parts, in which one part is originated in the removals of positive and negative ions to the opposite directions each other, and another the charge distribution induced by the electron. The decrease of the dielectric constants with increasing pressure is considered due to the more increasing of the repulsive overlap constant. Namely the hindrances for the removals of ions by the compressions of ionic crystals are considered to be the most effective factor for the decrease of the dielectric constants. On the other hand, the ions and the charge distribution should be strained with the increased lattice imperfection produced by deformation. Consequently, the polarization with the removals of ions and the electrons of ions may be disturbed by the imperfection.

The reflection spectra corresponding to restrahlen of TlCl in the region near the fundamental optical frequency are not affected by the plastic deformation. By this phenomena, it is considered that the fundamental optical mode of vibration and the damping for the lattice vibration are not affected by the plastic deformation. But, the effect of deformation are found in the side band of the reflection of NaF. The similar side band have been found in the reflection of ionic crystal having the ions of small masses, and considered to be the results of the interaction of the lattice vibration. By the combinations of the lattice vibrations, whose frequencies are ωt and ω respectively, a new mode of vibrations, whose frequency is $\omega t \pm \omega$ should be induced, and then the side band should be considered to be originated in this induced combination vibration.

As shown in the introduction in this paper, the three models have been considered for the explanation of the interaction of lattice vibrations. The possibility that structure might be at least partly associated with the presence of second order electric moments was suggested by Lax and Burstein[1]. At the present time it is known whether these moments contribute to the absorption in alkali halide where anharmonic effect is believed to be large. And, the increase of lattice imperfections by deformation is considered to have effect on the anharmonic effect of the lattice vibration.

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